MA 18: Topical session: Caloric Effects in ferroic materials I - Magnetocalorics

Time: Tuesday 10:15–11:45 Location: H53

MA 18.1 Tue 10:15 H53

The coupling of electronic, magnetic and lattice degrees of freedom in the magnetocaloric system La-Fe-Si — •Markus E. Gruner[1,2], Werner Keune[1], Beatriz Roldan Cuenya[3], Claudia Weis[1], Joachim Landers[1], Soma Salamon[1], Benedikt Eggert[1], Sergey I. Makarov[1], David Klar[1], Michael Y. Hu[4], Ercan E. Alp[4], Jiyong Zhao[4], Maria Krautz[5], Oliver Gutfleisch[6], and Heiko Wende[1] — [1]Universität Duisburg-Essen — [2]Forschungs-Neutronenquelle FRM II, Garching — [3]Ruhr-Universität Bochum — [4]Argonne National Laboratory — [5]IFW Dresden — [6]TU Darmstadt

$LaFe_{13-x}Si_x$ counts in its hydrogenated form as one of the most promising magnetocaloric materials for application. By combination of nuclear resonant inelastic X-ray scattering and first-principles calculations in the framework of density functional theory, we could recently demonstrate an unexpected phonon softening at the magnetic phase transition of pure La-Fe-Si, which contributes cooperatively with the magnetic degrees of freedom to the large magnetocaloric effect. The softening is traced back to adiabatic electron phonon coupling which originates from specific changes in the electronic density of states at the Fermi Level due to the itinerant electron metamagnetism of Fe [1]. Within this contribution we will review the signatures of itinerant electron metamagnetism and its implication for the magnetoelastic coupling in pure, Mn-doped and hydrogenated La-Fe-Si. Funding by the DFG (SPP1599, TRR80) is gratefully acknowledged.

[1] M. E. Gruner, W. Keune, B. Roldan Cuenya *et al.*, Phys. Rev. Lett. 114, 057202 (2015)

MA 18.2 Tue 10:45 H53

Element-resolved vibrational dynamics and thermodynamics of magnetocaloric FeRh compound — •Werner Keune[1], Markus E. Gruner[1], Joachim Landers[1], Soma Salamon[1], Franziska Scheibel[1], Detlef Spoddig[1], Beatriz Roldan Cuenya[2], Oliver Gutfleisch[3], Michael Y. Hu[4], Jiyong Zhao[4], Thomas Toellner[4], Ercan E. Alp[4], and Heiko Wende[1] — [1]Universität Duisburg-Essen, Germany — [2]Ruhr-Universität Bochum, Germany — [3]TU Darmstadt, Germany — [4]Argonne National Laboratory, USA

Employing both 57Fe nuclear resonant inelastic X-ray scattering and first principles calculations (DFT), similar to ref. [1], we determined the Fe-projected phonon DOS of the B2-ordered magnetocaloric FeRh compound at temperatures below and above the first-order magnetostructural phase transition from the antiferromagnetic (AFM) to the ferromagnetic (FM) state. Two experimental 57FeRh(001) thin-film samples on MgO(001) with different stoichiometries (AFM and FM, respectively) were studied. Distinct differences between the phonon DOS of the AFM and FM states were found. However, this leads only to very small differences in the T-dependences of the Fe-projected vibrational (lattice) specific heat C(T) and the vibrational entropy S(T), respectively, for the two magnetic states. The experimental Debye-Waller factor indicates that the lattice of the AFM state is softer than in the FM state.

[1] M. E. Gruner et al., Phys. Rev. Lett. 114, 057202 (2015).

MA 18.3 Tue 11:00 H53

Understanding the magnetostructural transitions of first-order materials — •Tino Gottschall, Dimitri Benke, Konstantin Skokov, Maximilian Fries, Iliya Radulov, and Oliver Gutfleisch — TU Darmstadt, Material Science, Darmstadt, Germany

The large magnetocaloric effect in the most promising first-order materials like La-Fe-Si [1], Fe2P type materials [2] or Heusler alloys [3] originates in the strong change of the magnetization with temperature being associated with a structural transformation. All these materials have one thing in common. The so-called magnetostructural transition goes hand in hand with a large volume change or at least a large change of the c to a ratio of the crystal structure.

In this work we present magnetic measurements of micrometer sized single particles of the three mentioned materials and compare them with the transformation characteristics of the corresponding bulk properties. It turns out that a very different behavior is observed depending on the size of the magnetocaloric sample. This result is of great importance for the application of magnetic refrigeration, especially for the design of powder bed heat exchangers.

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[1] I.A. Radulov, K.P. Skokov, D.Yu. Karpenkov, T. Gottschall, O. Gutfleisch, J. Mag. Mag. Mater. 396 (2015) 228 [2] F. Guillou, H. Yibole, G. Porcari, L. Zhang, N.H. van Dijk, E. Brück, J. Appl. Phys. 116 (2014) 063903 [3] T. Gottschall, K.P. Skokov, B. Frincu, O. Gutfleisch, Appl. Phys. Lett. 106 (2015) 021901

MA 18.4 Tue 11:15 H53

Complex magnetic intermetallics and magnetocaloric effect — •Peter Entel1 — Faculty of Physics and CENIDE, University of Duisburg-Essen, 47048 Duisburg, Germany

We have performed ab initio electronic structure calculations and Monte Carlo simulations of magnetic intermetallics such as Fe-Al, Fe-Rh, Ni-Mn-Ga and Ni-Mn-(In, Sn) alloys. While Fe-Al shows mictomagnetic and metamagnetic features due to disorder and defects, near-stoichiometric Ni-Mn-Ga alloys show magnetic-field induced strain (MFIS), as the external magnetic field can drive the variant boundaries to move so that the magnetic easy axis is aligned parallel to the magnetic field direction. The other unusual type of ferroic shape-memory alloys like Ni-Mn-(In, Sn) (showing large magnetocaloric effects) leads to strongly frustrated magnetic behavior because of competing ferro- and antiferromagnetic interactions, where the parent phase shows considerably larger magnetization than the martensitic phase leading (in difference to Ni-Mn-Ga) to magnetic field-induced transformation (MFIT), namely a metamagnetic phase transition from martensite to austenite with increasing magnetic field. The related magnetostructural transiton leads to the kinetic arrest phenomenon at a critical temperature where the entropy difference between austenitic and martensitic phases and the driving force for further transformation vanish (which, alternatively has been assigned to a Kauzmann point). In addition, we find transitions to supercooled austenite and unfrozen strain glass and to a cluster-spin glass. We argue that this complexity originates from the ferroic frustration and noncollinear magnetism.

15 min. coffee break